Coupled Core-Edge Simulations of Pedestal Formation Using the FACETS Framework

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Abstract. We present coupled core-edge simulations of pedestal buildup in the DIII-D tokamak using the FACETS framework. The FACETS project provides computational flexibility by allowing users to choose the best model for a given physics target. Our goals are to develop accurate transport solvers using neoclassical and turbulent fluxes with varying degree of fidelity and computational complexity, including embedded gyrokinetic simulations. Accurate sources using both ICRH wave absorption and neutral beam injection are included using parallel source components. Detailed modeling of the plasma edge using a fluid-based physics component, UEDGE, is performed and coupled to the core solver. The core region is simulated using a newly developed parallel, nested-iteration based non-linear solver while the UEDGE uses nonlinear solves from the PETSc/SNES solver package. With this new capability, simulations of DIII-D shots 118897 and 98889 are presented and compared to experiments. For this modeling, the core fluxes are computed from GLF23, NCLASS and Horton-ETG models. Sources are taken either from an interpretive ONETWO simulation or from a self-consistent NUBEAM simulation. The sensitivity of pedestal buildup to chosen transport models it studied. The effect of wall out-gassing on the core fueling and density buildup in the pedestal is discussed.

1. Introduction

To maximize return on investments in fusion experiments such as ITER, it is critical to develop and apply advanced computational tools not only to optimize design but also provide insights into experimental results. However, computational modeling of fusion plasmas remains a formidable challenge due to the wide range of time scales involved. Although accurate, solving the full kinetic equations is not practical for simulations of realistic long discharges. The FACETS project is the first significant effort aimed at combining the aspects of multi-physics and multiple computational regions (core, edge, and wall) within a single executable. We provide computational flexibility by allowing users to choose the best model for a given physics target. Our goals are to develop accurate transport solvers using neoclassical and turbulent fluxes with varying degree of fidelity and computational complexity, including embedded gyrokinetic simulations, accurate sources using both ICRH wave absorption and neutral beam injection, and improved boundary conditions by detailed modeling of the plasma edge and the tokamak wall.

The complexity of whole-device simulations of tokamaks translates to requiring a software component approach, as FACETS is taking. FACETS is bringing together successively more accurate and, hence, computationally demanding components to model the complete plasma device. It is being developed to run on LCFs to be able to use the most computationally demanding components, while at the same time it is usable on laptops for less demanding models. FACETS is constructing a C++ framework for incorporating the best software packages and physics components. A description of the FACETS framework is given in[3] in which the component approach and description of key concepts in the framework is given.

In this paper we present results from coupled core-edge simulations of pedestal buildup in the DIII-D tokamak for a selected shot. The rest of the paper is organized as follows. We first describe the progress made in the FACETS project in converting legacy applications to work on LCFs, improving performance by algorithmic enhancements, coupling of realistic beam particle and energy sources and development of a new plasma-wall interaction module. We then describe the core and edge equations used in the analysis and also describe the coupling scheme to advance the coupled system self-consistently in time. We describe the shot (DIII-D shot 118897), initial conditions and edge interpretive analysis used in the calculations. Results are then presented and discussed. We then make some concluding remarks and indicate further work on modelling the core-edge physics more accurately.

2. Converting legacy applications to components for Leadership Class Facilities

Transforming legacy fusion applications/libraries to FACETS components suitable for Leadership Class Facilities (LCFs) requires *glue code* to connect the legacy application to the FACETS interface and a cross-compile build environment to produce a statically linked executable. We chose to target a static executable to make FACETS portable to the widest possible collection of current and future LCFs. Glue code translates FACETS interface calls to legacy application calls and performs tasks like language interoperability, unit conversions, and calculating aggregate quantities from mesh data. In the case of UEDGE, our fluid edge component, we had to replace Python-based glue code with a new approach because Python typically uses dynamically loadable libraries — not a static executable. For the neutral beams deposition code NUBEAM, C++ wrappers were written directly calling in the Fortran 90 code.

For a few of the legacy applications including UEDGE and NUBEAM, we provided new autoconf-based build systems. These systems were designed to support multiple types of builds, for example serial, parallel, and static and dynamic. These systems required some adjustments to perform correctly on LCF machines where the front-end nodes are different than the compute nodes.

3. Improving performance of components through algorithmic modifications

Recent work has focused on incorporating robust and scalable parallel nonlinear solvers from the PETSc library into UEDGE to solve the nonlinear system $f(u) = 0$, where u represents the vector of unknowns. We implemented complete functionality for fully implicit, parallel matrix-free Newton-Krylov solvers. The use of PETSc has allowed us to overcome a major bottleneck in the parallel implementation of UEDGE. Strong nonlinearities exist owing to ionization and recombination, and the equation set must be well preconditioned to use the efficient Newton-Krylov solver technique. Previously, we could not simultaneously advance plasma and neutrals in parallel because of a very limited block Jacobi algorithm for the parallel preconditioner.

Implementation of PETSc has opened an array of possible preconditioners ranging from Jacobi, additive Schwarz, and finally full LU, which now allows us to advance both ions and neutrals together. Furthermore, the PETSc "coloring" scheme for efficiently computing the full finite-difference preconditioning Jacobian in parallel gives further substantial savings.

4. Coupling realistic particle and energy sources

The parallelized PPPL Monte Carlo package (NUBEAM) is used for computing the core sources from neutral beam injection. Progress in incorporating NUBEAM into FACETS has been made on two fronts: (i) design and development of a Plasma State physics component interface in Fortran and a mechanism to access this interface from a C/C++ driver and (ii) development of a parallelized driver for the NUBEAM component.

The strategy for coupling NUBEAM to a C/C++ driver leverages the Plasma State Component interface to NUBEAM that was already under development for the SWIM SCIDAC. The Plasma State (PS) is a fortran-90 object incorporating a time slice representation of a tokamak equilibrium, plasma profiles such as temperatures, densities, and flow velocities, and core plasma particle, momentum, and energy sources. It also incorporates a machine description section containing time invariant quantities such as neutral beam and RF antenna geometries. The PS implementing code along with the C/C++ wrapper is generated from a state specification file using a Python script.

A new parallelized driver for the NUBEAM has been developed. This has allowed testing, scaling studies, and served as a template for the C++ driver in FACETS. NUBEAM is the first component in FACETS using volumetric coupling with core transport equations.

5. Plasma-wall interaction module

The edge plasma and material wall are strongly coupled primarily via particle recycling, impurity production, and plasma power exhaust. The handling of transient and static peak power loads, core plasma contamination with impurities, plasma-facing components lifetime, and hydrogen retention in walls are the critical issues affecting the design of next-step fusion devices (like ITER, CTF, DEMO). To address these issues and to model self-consistently the plasma-wall coupling in FACETS, the Wall and Plasma-Surface Interactions (WALLPSI) module was developed[5].

The work on WALLPSI verification and validation against vast experimental data is in progress. Several laboratory experiments had showed clear saturation of retained deuterium in beryllium and in graphite (e.g. pyrolitic graphite). In[5], the results of simulations of static deuterium retention in graphite and beryllium at room temperatures with WALLPSI were presented showing good agreement with experimental data (see Fig. 1). Here, deuterium is retained via collisional production of broken bond traps followed by population of these traps by deuterium atoms. The modeled saturated dose for deuterium in graphite is consistent with [D]/[C]=0.4, the measured concentration of statically retained deuterium averaged over the projectile range. WALLPSI verification includes solving of simple diffusive 1-D transport problems for hydrogen in wall material.

The coupled plasma-wall modeling scheme with WALLPSI was tested by: (i) calculating the inventory build-up of mobile, chemically bonded, adsorbed and trapped hydrogen in the wall as well as the nonlinear variation of hydrogen recycling coefficient and impurity production rate in response to the incident plasma particle and energy fluxes, and (ii) simulating the spatiotemporal evolution of plasma parameters and hydrogen inventory in the wall with the coupled WALLPSI and plasma transport code EDGE1D for a range of plasma conditions[5].

6. Core and Edge Models and Coupling Scheme

High-performance tokamak plasma discharges (so-called "H-mode" plasmas) are characterized by steep gradients of temperature and density near the plasma separatrix where open field lines

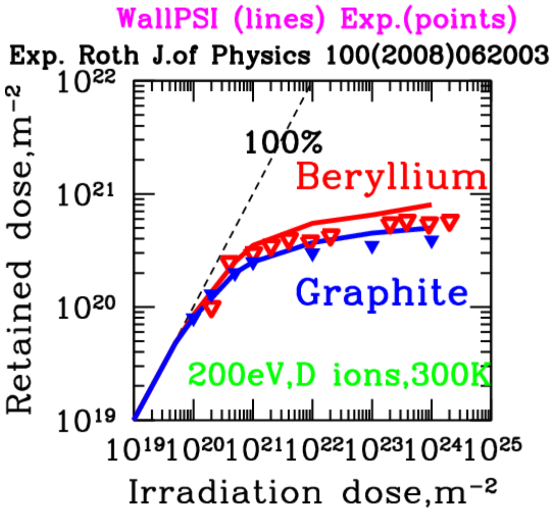

Figure 1. Example of WALLPSI validation against experimental retention data

separate from closed field lines. This region is referred to as the "H-mode pedestal". Experiments and core transport simulations indicate that core profiles are relatively insensitive to the overall values of density and temperature, but that the shape is set by stiff transport due to kinetic turbulence. Thus, the overall fusion gain depends sensitively on the parameters at the top of the pedestal temperature and density[4]. The pedestal height serves as a boundary condition to the core plasma region. The physics determining the formation of the pedestal (the so-called L-H transition) is not fully understood, and is the subject of active investigations[6]. As a first test of the FACETS code we have undertaken the simulation of the the pedestal buildup in a particular shot of the DIII-D tokamak. However, due to poor understanding of the edge physics and lack of availability of predictive models for the edge transport we have used an interpretive analysis to determine the edge cross-field transport coefficients. These are held constant throughout the simulation. Although not fully self-consistent, this serves to test the infrastructure and also gives insight into the time-scales over which edge transport coefficients evolve.

Well inside the separatrix the plasma is hot which leads to large disparities in the transport parallel and perpendicular to the field lines. This in turn implies that, on transport time-scales, the plasma equilibriates in the poloidal direction and the physics can now be described as a set of one dimensional equations for the perpendicular transport of density and energy

$$\frac{\partial n}{\partial t} + \frac{1}{V'}\frac{\partial}{\partial \rho}(V' F_n^{\rho}) = S_n \tag{1}$$

$$\frac{3}{2}\frac{\partial}{\partial t}(n T_s) + \frac{1}{V'}\frac{\partial}{\partial \rho}(V' F_s^{\rho}) = S_s \tag{2}$$

where $n(\rho, t)$ is the plasma number density, $T_s(\rho, t)$ are electron ($s = e$) and ion ($s = i$) temperatures, F_n^{ρ} is the contravariant particle flux, F_s^{ρ} are the contravariant thermal fluxes and $S_n(\rho, t)$ and $S_s(\rho, t)$ are the particle and thermal sources. The independent variable is the dimensionless normalized toroidal flux ρ and the radial geometry is encapsulated in $V' \equiv dV/d\rho$, where $V(\rho)$ is the volume enclosed inside the flux surface ρ.

The fluxes are computed using a combination of anomalous and neoclassical terms $F_{\mathrm{GLF}} + F_{\mathrm{CH}} + F_{\mathrm{ETG}}$, where F_{GLF} is the anomalous flux computed using the GLF23[7] model, F_{CH} is the neoclassical flux computed using the Chang-Hinton[8] model and F_{ETG} is anomalous electron transport due to Horton-ETG model[9]. The system of core transport equations Eq. (1) and

Eq. (2) are highly non-linear and stiff due to the strong dependence of the fluxes on the gradients of the density and temperatures. A nested-iteration based implicit solver is implemented in FACETS to evolve this set of equations. In[10] the FACETS solver is verified by comparison against the ASTRA code.

As we approach the separatrix the plasma cools and the field lines are no longer nested. This leads to two-dimensional effects and the plasma transport both along and perpendicular to the field lines now needs to be evolved. FACETS incorporates the fluid edge code UEDGE[11, 12] to solve the edge plasma equations. UEDGE includes full single- or double-null X-point geometry with a simulation domain including the region spanning well inside the separatrix and extending to the outer wall and the divertor plate region. A reduced set of the Braginskii transport equations is solved. Usually the cross diffusion terms are turned off and the Alfven waves are suppressed by not evolving the induction equation for the magnetic field. Additional assumptions are used to express the equations in a form more amenable to disabling various physics terms to allow faster solution times, or to allow better physics understanding. The specific form of the equations are found in Ref.[12].

The coupling between the core and the edge regions is performed using an explicit scheme. There are several challenges in setting up an self-consistent problem across the one-dimensional predictive core region with the two-dimensional interpretive edge region. First, the initial conditions need be to C^1 continuous across the core-edge (CE) interface. Second, the transport coefficients at the CE interface need to match. This is particularly difficult as completely different models are used to compute the fluxes in the core and edge solvers. An ad-hoc scheme is presently implemented in FACETS to enforce this. The continuity in the initial conditions is ensured by using the same set of experimental data to initialize both the core and the edge. However, this does not guarantee the continuity of slopes at the CE interface as two components use different grids and discretization schemes.

The coupled simulation is run as follows. The core and edge components are run concurrently for a specified time-step dt. Typically, both component need to sub-cycle to evolve their solutions by this time-step. The particle and energy fluxes are passed from the core to the edge, i.e. $F^\rho V'/A = F^\rho / < |\nabla\rho| >$ is sent to the edge, where A is the area of the flux surface at the CE interface and the angular brackets indicate flux surface averaging. The flux-surface averaged temperature and number density are passed from the edge to the core. These steps are repeated and the simulation evolved in time.

The explicit coupling scheme described above is stable as long as sufficiently small time-steps are taken. Numerical experiments show that a time-step on the order of several 100 μs can be taken without the coupled solution going unstable. A fully implicit coupling scheme, although not used in this paper, is also implemented in FACETS and presently being tested for use in core-edge simulations.

7. Problem Setup and Results

Coupled core-edge simulations using the methods described in the previous section are performed to study the pedestal buildup in the DIII-D tokamak. For this we have chosen to simulate the time slice from 1555 to 1590 ms of DIII-D shot 118897. From the experimental wave forms it is seen that the neutral beams are turned on around 1490 ms and the plasma density increases from around 2.8×10^{19} m^3 to 3.9×10^{19} m^3.The beam power in the chosen interval averages to around 4.5 MW and eventually drops down to 2.5 MW around 1600 ms. The discharge is ELM free till around 2355 ms.

Beam sources are held constant during the simulation and are taken from an interpretive ONETWO simulation. See Fig. 2 for beam source heating profiles for ions and electrons. The simulation is initialized using experimental data averaged around 1555 ms into the discharge. See Fig. 3 for initial density and temperature profiles. The core component is run to $\rho = 0.85$

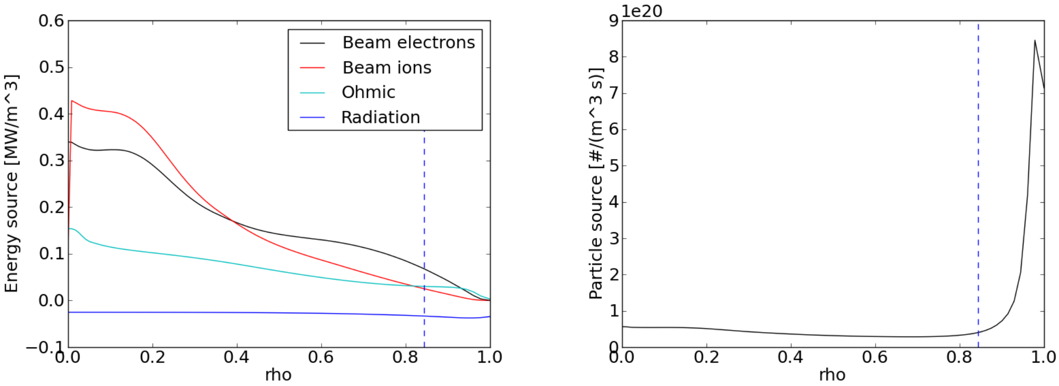

Figure 2. Power sources for electrons and ions (left) and plasma particle source (right). Total beam power for ions is 1.78 MW, for electrons 2.21 MW and Ohmic heating is 0.93 MW and radiation loss is 0.40 MW. Net particle injection rate is 2.12×10^{21} s^{-1}. Out of these, the fraction of particles into the core is 4.99×10^{20} s^{-1}. Rest (1.617×10^{21} s^{-1}) should be accounted for in the edge.

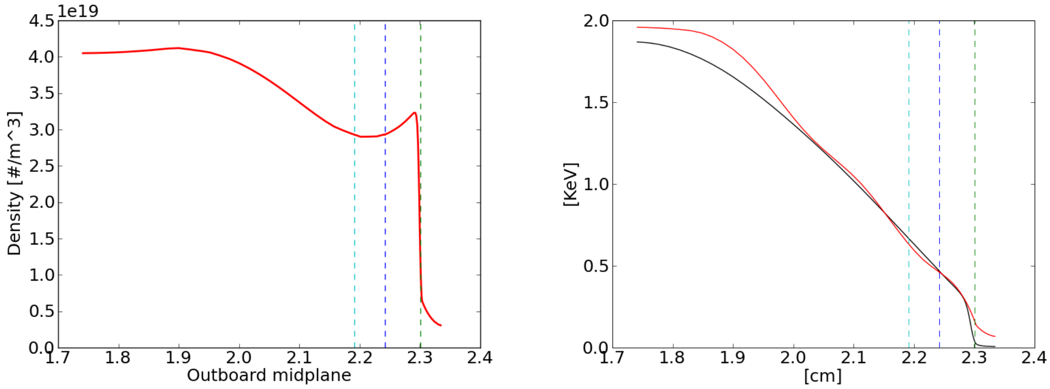

Figure 3. Initial density (left) and temperature (right) profiles for electrons (black) and ions (red) for shot 118897 at 1555 ms. The blue dashed lines indicate the core-edge interface, the green dashed line the separatrix and the cyan line the start of transition from predictive to interpretive fluxes.

and the edge component from there to the wall. Note that this puts the pedestal inside the edge component. The reason for doing this is two fold: (a) the core transport models do not work very well for $\rho > 0.85$ and, (b) we want to ensure that the edge is sufficiently inside the separatrix for the solutions to be relaxed along the poloidal direction.

An initial set of calculations using experimental profiles and sources is performed to determine the cross-field diffusivities for UEDGE. See Fig. 4. The diffusivites drop down significantly in the pedestal to create a transport barrier for the pedestal formation. As mentioned before this procedure is not self-consistent as the core is predictive, but lacking predictive edge models this method must be adopted. A fully interpretive edge model should predict a similar transport barrier. Once these diffusivities were determined they were held constant through the 35 ms simulation time.

The core and edge components were evolved using the explicit coupling scheme described above. A time-step of 200 μs was used to couple the components, although the components

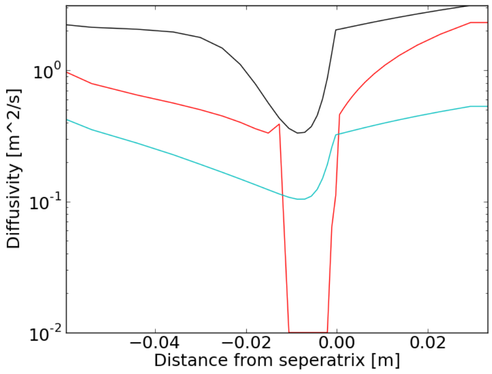

Figure 4. UEDGE diffusivities from interpretive calculations. Red line D, black line χ_e, blue line χ_i.

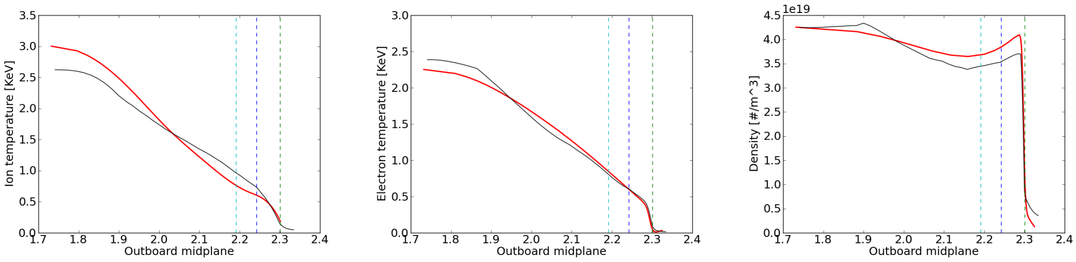

Figure 5. Final experimental (red) and simulation results (black) for ion (left) and electron (middle) temperatures at 35 ms. Final experimental density profile (red) and simulation results (black) are shown in the right panel. The ion temperature is over-predicted at the pedestal while the plasma density is under-predicted. Tuning the gas puff to supply an additional particle fueling source could lead to a higher density buildup in the edge.

internally were allowed to choose their own time-steps. Plasma density, electron and ion energy equations were evolved. See Fig. 5 for comparison between simulation results and experimental profiles averaged around 1590 ms into the discharge. Our initial results show that the electron temperature is predicted better that the ion temperature. As seen in the figure the ion pedestal temperature rises beyond that seen in the experiment, indicating a greater flow of ion thermal energy into the edge. This leads to a corresponding loss in ion energy near the magnetic axis. This is behaviour is being investigated and it is believed that a proper accounting for the $\omega_{|E\times B|}$ shear profile will lead to a damping to the ion thermal flux near the CE interface and improve the ion temperature predictions. It is also seen that the density buildup in the edge is under-predicted. The reason for this could be that the neutral particle source fueling the edge is not sufficient to supply the net line-integrated density in the tokamak. An additional gas-puff source would supply this particle source and this is being investigated at present.

8. Conclusions

We have presented coupled core-edge simulations of pedestal buildup in a selected shot of the DIII-D tokamak. Our initial simulations show that FACETS can evolve the plasma density in addition to the electron and ion energy equations self-consistently using coupled core-edge simulations. Our initial calculations have shown a sensitivity of the pedestal buildup on the core-edge power balance and also to the presence of a gas-puff as a fueling source in the edge. These calculations show the ability of the framework to perform concurrent coupled simulations with multiple components and serve as a test for the explicit coupling algorithms. We expect improvements in the predicted ion temperature and plasma density with a better accounting of the shear flow profiles and a proper tuning of the gas-puff. We believe that our agreement with experiments is reasonable given the uncertainties in the core density model (GLF23) and the lack of a predictive edge model.

Our current work in FACETS is to increase the physics fidelity of the simulations. We have incorporated the NUBEAM neutral beams package that allows the self-consistent computation of the beam deposition into the core. However, before NUBEAM can be used on a production level it will have to be extended to deposit power into the edge. We have incorporated the TGLF[13] anomalous transport model to better predict the core transport coefficients. We have implemented a Newton-method based implicit coupling algorithm that we expect will allow us to take 10 ms time-steps, thus increasing the discharge time that can be simulated. We have completed the implementation of a sophisticated wall model that will be incorporated into the simulations. FACETS is now being used to simulate other DIII-D discharges to better quantify the core-edge physics.

References

[1] U. D. of Energy, “Facilities for the future of science: A twenty-year outlook.” `http://www.er.doe.gov/about/Future/Facilities\for\the\Future\of\Science.htm`, 2003.

[2] J R Cary, J Candy, R H Cohen, S Krasheninnikov, D C McCune, D J Estep, J Larson, A D Malony, A. Pankin *et al* 2008 First results from core-edge parallel composition in the FACETS project *J. Physics: Conf. Series* **125** 012040

[3] John R. Cary, Ammar Hakim, Mahmood Miah, Scott Kruger, Alexander Pletzer, Svetlana Shasharina, Srinath Vadlamani, Alexei Pankin, Ronald Cohen, Tom Epperly, Tom Rognlien, Richard Groebner, Satish Balay, Lois McInnes, Hong Zhang, ”FACETS - a Framework for Parallel Coupling of Fusion Components”, *The 18th Euromicro International Conference on Parallel, Distributed and Network-Based Computing.* Pisa, Italy. 2010.

[4] J. Kinsey, G. Staebler, and R. Waltz, “Burning plasma confinement projections and renormalization of the GLF23 drift-wave transport model,” *Fus. Sci. Tech.*, vol. 44, p. 763, 2003.

[5] A.Yu. Pigarov and S.I. Krasheninnikov, Coupled plasma-wall modeling, *Journal Nuclear Materials* **390-391** (2009) 192.

[6] R. Groebner, A. Leonard, P. Snyder, T. Osborne, C. Maggi, M. Fenstermacher, C. Petty, and L. Owen, “Progress towards a predictive model for pedestal height in diii-d,” *Nucl. Fusion*, vol. 49, p. 085037, Jul 2009.

[7] J. E Kinsey and G. M Staebler and R. E Waltz, “Predicting core and edge transport barriers in tokamaks using the GLF23 drift-wave transport model”, *Physics of Plasmas*, vol 12 (15), p. 052503, 2005.

[8] C. S. Chang and F. L Hinton, “Effect of impurity particles on the finite-aspect ratio neoclassical thermal conductivity in a tokamak”, *Physics of Fluids*, vol 29 (10), p. 3314–3316, 1986.

[9] T Rafiq, AY Pankin, G Bateman and A. H Kritz F. D Halpern, “Simulation of electron thermal transport in H-mode discharges”, *Physics of Plasmas*, vol 16, p. 032505, 2009.

[10] Alexei Y. Pankin, Alex Pletzer, Srinath Vadlamani, John R. Cary, Ammar Hakim, Scott E. Kruger, Mahmood Miah, Thomas D. Rognlien, Svetlana Shasharina, Glenn Bateman, Arnold H. Kritz, and Tariq Rafiq. Simulation of anomalous transport in tokamaks using the FACETS code. *Computer Physics Communications*, In Press, Corrected Proof 2010. (doi: 10.1016/j.cpc.2010.07.03)

[11] T. Rognlien, J. Milovich, M. Rensink, and G. Porter, “A fully implicit, time dependent 2-d fluid code for modeling tokamak edge plasmas,” *Journal of Nuclear Materials*, vol. 196–198, pp. 347–351, 1992.

[12] Thomas D Rognlien, Dmitri D Ryutov, N Mattor, and G. D Porter. Two-dimensional electric fields and drifts near the magnetic separatrix in divertor tokamaks. *Physics of Plasmas*, 6:1851, 1999.

[13] G M Staebler, J.E Kinsey, and R.E Waltz. A theory-based transport model with comprehensive physics. *Physics of Plasmas*, 14:055909, May 2007.